



22<sup>nd</sup> International Conference on  
Diffusion in Solids and Liquids  
22 TO 26 JUNE 2026 | RHODES, GREECE

## ABSTRACT:

### Interface Phases: a Design Tool Across Material Systems

C.H. Liebscher<sup>1,2</sup>

<sup>1</sup>Faculty of Physics and Astronomy, Ruhr University Bochum, Bochum, Germany

<sup>2</sup>Research Center Future Energy Materials and Systems, Ruhr University Bochum, Germany

Interfaces in crystalline materials are not merely structural defects but can host distinct structural phases with properties fundamentally different from those of the adjoining bulk crystals. These interface phases emerge from broken symmetry, excess thermodynamic quantities, and locally altered bonding environments, giving rise to structures and electronic states that are inaccessible in the bulk.

In this talk, we illustrate how multiple structural states can coexist at grain boundaries and transform into one another under external stimuli such as temperature or changes in composition. Combining atomic-resolution scanning transmission electron microscopy with atomistic modeling, we demonstrate that grain boundaries can adopt structurally and chemically distinct states, separated by well-defined phase junctions. From this perspective, we outline the general structural and thermodynamic principles governing grain boundary phase transformations and identify common concepts that extend across both structural and functional material systems.

Building on this foundation, we highlight the broader implications of interface phases as a new degree of freedom in materials design. The deliberate control of interfacial states—and their transformations—suggests a shift toward a paradigm in which functionality can be engineered through interface states. As a concrete example, we discuss heterogeneous catalytic systems, where grain boundaries in Au nanoassemblies play a decisive role in governing catalytic activity and stability.